

Pentane, 2-iodo-

Other names:	2-Iodopentane Pentane, 2-iodo-, (.+/-.)- s-Amyliodide sec-Amyl Iodide
Inchi:	InChI=1S/C5H11I/c1-3-4-5(2)6/h5H,3-4H2,1-2H3
InchiKey:	JUPBFIYJUCWJCT-UHFFFAOYSA-N
Formula:	C5H11I
SMILES:	CCCC(C)I
Mol. weight [g/mol]:	198.05
CAS:	637-97-8

Physical Properties

Property code	Value	Unit	Source
gf	46.90	kJ/mol	Joback Method
hf	-74.94	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	35.71	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.610		Crippen Method
mcvol	107.130	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
ripol	873.00		NIST Webbook
ripol	873.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1177.00		NIST Webbook
tb	406.50	K	Joback Method
tc	613.94	K	Joback Method
tf	189.17	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.15	J/mol×K	406.50	Joback Method
cpg	182.14	J/mol×K	441.07	Joback Method
cpg	191.61	J/mol×K	475.65	Joback Method
cpg	200.59	J/mol×K	510.22	Joback Method
cpg	209.09	J/mol×K	544.79	Joback Method
cpg	217.13	J/mol×K	579.36	Joback Method
cpg	224.75	J/mol×K	613.94	Joback Method
dvisc	0.0102765	Paxs	189.17	Joback Method
dvisc	0.0037890	Paxs	225.39	Joback Method
dvisc	0.0018416	Paxs	261.61	Joback Method
dvisc	0.0010668	Paxs	297.84	Joback Method
dvisc	0.0006956	Paxs	334.06	Joback Method
dvisc	0.0004932	Paxs	370.28	Joback Method
dvisc	0.0003718	Paxs	406.50	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37212e+01
Coeff. B	-3.37291e+03
Coeff. C	-5.68400e+01
Temperature range (K), min.	307.92
Temperature range (K), max.	457.91

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C637978&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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